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NUMERICAL SIMULATIONS OF CLUSTER FORMATION USING A DISCRETE VELOCITY KINETIC THEORY OF GASES

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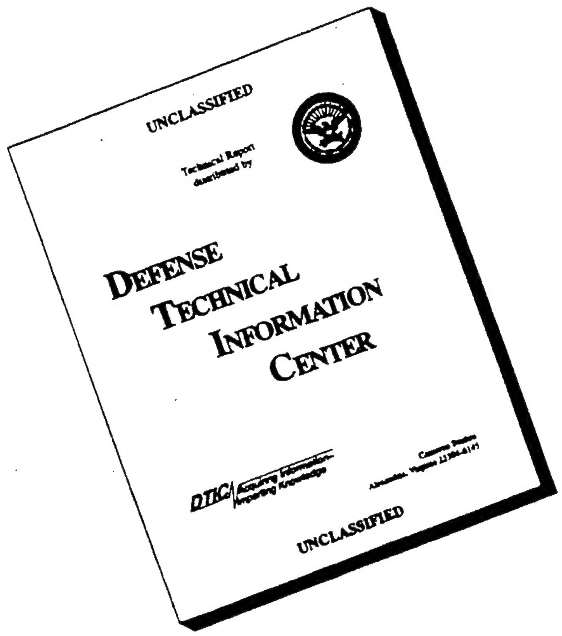

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NUMERICAL SIMULATIONS OF CLUSTER FORMATION USING A DISCRETE VELOCITY KINETIC THEORY OF GASES

M. Slemrod and A. Qi

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ABSTRACT

Cluster formation is simulated numerically with discrete velocity Boltzmann model in two space dimensions. The model exhibits cluster coagulation, fragmentation, and transport. It evolves on two different scales obtained from an elastic and inelastic collision Knudsen numbers ε and μ respectively. For flow impinging on a wall with specularly reflective boundary condition these scales appear both analytically and numerically.

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§1 Introduction

In recent paper Slemrod, Grinfeld, Qi and Stewart [8] have given a model and one dimensional numerical simulation for a discrete velocity gas exhibiting coagulation and fragmentation. For example such a model might illustrate same of the grosser features of nucleating droplets that make up fog or an aerosol.

The model is based on the rules of discrete velocity kinetic theory and many of the ideas using in developing the model are to be found in an earlier model of Monaco and Pandolfi Bianchi [2, 3]. The new feature of the model of [8] is that it allows clusters of particles with unlimited cluster size while the model [2] did not.

The model of [8] contains two length scales based on an elastic Knudsen number ε and inelastic Knudsen number μ. Since inelastic collision processes proceed much slower than elastic ones we expect $0 < \varepsilon << \mu$. This in turn implies at least for steady flow that we should see different regimes of gas flow in a neighborhood of a boundary.

In this paper we consider this issue analytically and numerically. Indeed in a sequence of photos of computer generated data we have able to see the boundary layers rather sharply completely consistent with the analytical analysis.

§2 The discrete velocity coagulation-fragmentation model

We consider a discrete velocity gas of identical particles each of mass m contained in volume $V \subseteq R^3$. A point in V is identified with its Euclidean coordinates (x, y, z). The particles are grouped into clusters possessing $1, 2, ..., M$ particles where the cluster of size M is the largest cluster that can be crammed into V. The clusters move in V with fixed momenta

$\underline{P}_1 = m(c,0,0)$, $\underline{P}_2 = m(-c,0,0)$, $\underline{P}_3 = m(0,c,0)$, $\underline{P}_4 = m(0,-c,0)$, $\underline{P}_5 = m(0,0,c)$, $\underline{P}_6 = m(0,0,-c)$, $\underline{P}_0 = m(0,0,0)$. A cluster made up of α-particles will be called an α-cluster. It is clear that an α-cluster with momentum $\underline{P}_j$ has velocity $\underline{v}_j^\alpha = \frac{\underline{P}_j}{m\alpha}$.

As the clusters move in V they collide in a binary fashion. Both elastic and inelastic collisions are allowed. In terms of the momenta $\underline{P}_i$ the elastic collisions will be represented by list $\underline{P}_1 + \underline{P}_2 = \underline{P}_3 + \underline{P}_4 = \underline{P}_5 + \underline{P}_6$ while the inelastic collisions are defined by $\underline{P}_1 + \underline{P}_2 = \underline{P}_0$, $\underline{P}_3 + \underline{P}_4 = \underline{P}_0$, $\underline{P}_5 + \underline{P}_6 = \underline{P}_0$, $\underline{P}_i + \underline{P}_0 = \underline{P}_i$ $(i = 1, ..., 6)$. Notice elastic collisions conserve mass, momentum, and energy; inelastic collisions conserve mass and momentum but not energy. We denote by $n_j^\alpha(x,y,z,t)$ the number density of α-clusters with momentum $\underline{P}_j$ at a point $(x,y,z) \in V$ at time $t > 0$, i.e. the number of clusters in this class per unit volume.

A collision of an α-cluster with momentum $\underline{P}_i$ and a β-cluster with momentum $\underline{P}_j$ which yields a δ-cluster with momentum $\underline{P}_k$ and a γ-cluster with momentum $\underline{P}_\ell$ will be represented by $(n_i^\alpha, n_j^\beta) \rightarrow (n_k^\delta, n_\ell^\gamma)$. This notation allows us to write the allowable elastic collisions as follows.

1. Mechanical collisions: $(n_1^\alpha, n_2^\alpha) \rightarrow (n_1^\alpha, n_2^\alpha)$ $(prob.\frac{1}{3})$, (n_3^α, n_4^α) $(prob.\frac{1}{3})$, (n_5^α, n_6^α) $(prob.\frac{1}{3})$ with similar statements for (n_3^α, n_4^α), (n_5^α, n_6^α).

2. Exchange collisions: (a) "head-on" collisions: $(n_1^\alpha, n_2^\beta) \rightarrow (n_1^\alpha, n_2^\beta)$ $(prob.\frac{1}{6})$, (n_1^β, n_2^α) $(prob.\frac{1}{6})$, (n_3^α, n_4^β) $(prob.\frac{1}{6})$, (n_3^β, n_4^α) $(prob.\frac{1}{6})$, (n_5^α, n_6^β) $(prob.\frac{1}{6})$, (n_5^β, n_6^α) $(prob.\frac{1}{6})$ with similar statements for (n_3^α, n_4^β) and (n_5^α, n_6^β). (b) "angle" collisions: $(n_1^\alpha, n_3^\beta) \rightarrow (n_1^\alpha, n_3^\beta)(prob.\frac{1}{2})$, (n_1^β, n_3^α) $(prob.\frac{1}{2})$ with similar statements for (n_1^α, n_5^β) and (n_3^α, n_5^β).

We only allow inelastic collisions of the Becker-Döring type [4, 5, 7], i.e. where an α-cluster may gain or lose a 1-cluster in coagulation or fragmentation respectively. The

coagulation of a 1-cluster with momentum $\underline{P}_j$ to form an $\alpha+1$-cluster with momentum $\underline{P}_k$ is represented as $(n_i^1, n_j^\alpha) \rightarrow (n_k^{\alpha+1})$ while the fragmentation of an $\alpha+1$-cluster with momentum $\underline{P}_k$ into a 1-cluster with momentum $\underline{P}_i$ and an α-cluster with momentum $\underline{P}_j$ will be denoted by $(n_k^{\alpha+1}) \rightarrow (n_i^1, n_j^\alpha)$. With this notation the allowable Becker-Döring inelastic collisions are as follows.

1. "Head on" coagulation: $(n_1^1, n_2^{\alpha-1})$, $(n_1^{\alpha-1}, n_2^1)$, $(n_3^1, n_4^{\alpha-1})$, $(n_3^{\alpha-1}, n_4^1)$, $(n_5^1, n_6^{\alpha-1})$, $(n_5^{\alpha-1}, n_6^1) \rightarrow (n_0^\alpha)$.

2. "Moving cluster coagulates with rest cluster": $(n_j^1, n_0^{\alpha-1})$, $(n_j^{\alpha-1}, n_0^1) \rightarrow n_j^\alpha$, $j = 1, 2, ..., 6$.

3. Reversal of 1 (fragmentation): $(n_0^\alpha) \rightarrow (n_1^1, n_2^{\alpha-1})(prob.\frac{1}{6})$, $(n_1^{\alpha-1}, n_2^1)\ (prob.\frac{1}{6})$, $(n_3^1, n_4^{\alpha-1})$ $(prob.\frac{1}{6})$, $(n_3^{\alpha-1}, n_4^1)\ (prob.\frac{1}{6})$, $(n_5^1, n_6^{\alpha-1})\ (prob.\frac{1}{6})$, $(n_5^{\alpha-1}, n_6^1)\ (prob.\frac{1}{6})$ if $\alpha > 2$; $(n_0^2) \rightarrow (n_1^1, n_2^1)\ (prob.\frac{1}{3})$, (n_3^1, n_4^1), $(prob.\frac{1}{3})$, $(n_5^1, n_6^1)\ (prob.\frac{1}{3})$.

4. Reversal of 2 (fragmentation): $(n_j^\alpha) \rightarrow (n_j^1, n_0^{\alpha-1})\ (prob.\frac{1}{2})$, $(n_0^1, n_j^{\alpha-1})\ (prob.\frac{1}{2})$, $j = 1, 2, ..., 6$ if $\alpha > 2$; $(n_j^2) \rightarrow (n_j^1, n_0^1), j = 1, 2, ..., 6$.

The rate equations governing the motion of clusters are given by the transport equations

$$
\begin{aligned}
\frac{\partial n_1^\alpha}{\partial t} + \frac{c}{\alpha}\frac{\partial n_1^\alpha}{\partial x} &= E_1^\alpha + I_1^\alpha\,, \\
\frac{\partial n_2^\alpha}{\partial t} - \frac{c}{\alpha}\frac{\partial n_2^\alpha}{\partial x} &= E_2^\alpha + I_2^\alpha\,, \\
\frac{\partial n_3^\alpha}{\partial t} + \frac{c}{\alpha}\frac{\partial n_3^\alpha}{\partial y} &= E_3^\alpha + I_3^\alpha\,, \\
\frac{\partial n_4^\alpha}{\partial t} - \frac{c}{\alpha}\frac{\partial n_4^\alpha}{\partial y} &= E_4^\alpha + I_4^\alpha\,, \quad 1 \le \alpha \le M \qquad (2.1) \\
\frac{\partial n_5^\alpha}{\partial t} + \frac{c}{\alpha}\frac{\partial n_5^\alpha}{\partial z} &= E_5^\alpha + I_5^\alpha\,,
\end{aligned}
$$

$$\frac{\partial n_6^\alpha}{\partial t} - \frac{c}{\alpha}\frac{\partial n_6^\alpha}{\partial z} = E_6^\alpha + I_6^\alpha \ ,$$
$$\frac{\partial n_0^\alpha}{\partial t} = I_0^\alpha \ .$$

The calculation of E_j^α has been given in [2, 3] according to the rules of discrete velocity kinetic theory, i.e. these terms are proportional to collisional cross sectional areas; the relative velocity of the particles before collision; the probability of each admissible collision; both number densities of the colliding particles. Clearly $E_0^\alpha = 0, \alpha = 1, ..., M$. We record the rest of E_j^α and the inelastic collision terms I_j^α in Appendix.

It is a straightforward exercise to show

$$E_1^\alpha + E_2^\alpha + E_3^\alpha + E_4^\alpha + E_5^\alpha + E_6^\alpha = 0 \ , \ \alpha = 1, ..., M \ ,$$
$$\sum_{\alpha=1}^{M} E_1^\alpha - E_2^\alpha = \sum_{\alpha=1}^{M} E_3^\alpha - E_4^\alpha = \sum_{\alpha=1}^{M} E_5^\alpha - E_6^\alpha = 0 \ ,$$
$$\sum_{\alpha=1}^{M} \alpha (I_0^\alpha + I_1^\alpha + I_2^\alpha + I_3^\alpha + I_4^\alpha + I_5^\alpha + I_6^\alpha) = 0 \ ,$$
$$\sum_{\alpha=1}^{M} I_1^\alpha - I_2^\alpha = \sum_{\alpha=1}^{M} I_3^\alpha - I_4^\alpha = \sum_{\alpha=1}^{M} I_5^\alpha - I_6^\alpha = 0 \ .$$

Next define the quantity:

$$\begin{aligned}
J_\alpha \ = \ & n_0^\alpha (a_{\alpha,1}^{1,0} n_1^1 + a_{\alpha,1}^{2,0} n_2^1 + a_{\alpha,1}^{3,0} n_3^1 + a_{\alpha,1}^{4,0} n_4^1 + a_{\alpha,1}^{5,0} n_5^1 + a_{\alpha,1}^{6,0} n_6^1) \\
& + (1 - \delta_{\alpha 1}) n_0^1 (a_{\alpha,1}^{1,0} n_1^\alpha + a_{\alpha,1}^{2,0} n_2^\alpha + a_{\alpha,1}^{3,0} n_3^\alpha + a_{\alpha,1}^{4,0} n_4^\alpha + a_{\alpha,1}^{5,0} n_5^\alpha + a_{\alpha,1}^{6,0} n_6^\alpha) \\
& + (1 - \delta_{\alpha 1})(a_{\alpha,1}^{1,2} n_1^\alpha n_2^1 + a_{\alpha,1}^{3,4} n_3^\alpha n_4^1 + a_{\alpha,1}^{5,6} n_5^\alpha n_6^1) \\
& + a_{\alpha,1}^{2,1} n_2^\alpha n_1^1 + a_{\alpha,1}^{4,3} n_4^\alpha n_3^1 + a_{\alpha,1}^{6,5} n_6^\alpha n_5^1 \\
& - b_{\alpha+1}^1 n_1^{\alpha+1} - b_{\alpha+1}^2 n_2^{\alpha+1} - b_{\alpha+1}^3 n_3^{\alpha+1} - b_{\alpha+1}^4 n_4^{\alpha+1} \\
& - b_{\alpha+1}^5 n_5^{\alpha+1} - b_{\alpha+1}^6 n_6^{\alpha+1} \qquad \text{for } 1 \le \alpha \le M - 1 \ , \\
J_M \ = \ & 0 \ .
\end{aligned}$$

It then follows that

$$I_0^\alpha + I_1^\alpha + I_2^\alpha + I_4^\alpha + I_5^\alpha + I_6^\alpha = J_{\alpha-1} - J_\alpha \ , \ 1 \le \alpha \le M \ .$$

Let us define

$$n_j^\alpha = \bar{n}_j^\alpha \mathcal{R}$$

where $\mathcal{R}$ is a typical value of the density $\sum_{j=0}^{6} \sum_{\alpha=1}^{M} \alpha n_j^\alpha$, $x = \bar{x}L$, $y = \bar{y}L$, $z = \bar{z}L$, $ct = \bar{t}L$ where L is a typical macroscopic length. Hence $\bar{n}_j^\alpha$, $\bar{x}$, $\bar{y}$, $\bar{z}$ are dimensionless quantities. Then for example in equation (2.1) we see

$$\frac{\partial \bar{n}_1^\alpha}{\partial \bar{t}} + \frac{1}{\alpha} \frac{\partial \bar{n}_1^\alpha}{\partial \bar{x}} = \frac{L}{c\mathcal{R}} (E_1^\alpha + I_1^\alpha).$$

Hence we see

$$\frac{\partial \bar{n}_1^\alpha}{\partial \bar{t}} + \frac{1}{\alpha} \frac{\partial \bar{n}_1^\alpha}{\partial \bar{x}} = L r_1^2 \mathcal{R} (\bar{E}_1^\alpha) + \frac{L}{c\mathcal{R}} I_1^\alpha,$$

where we define $\bar{E}_1^\alpha$ as E_1^α with $c = 1$, n_j^α replaced by $\bar{n}_j^\alpha$, and $r_1 = 1$ in the definition of $\sigma_{\alpha\beta}$. Next set $\varepsilon = 1/L r_1^2 \mathcal{R}$ which is the dimensionless elastic Knudsen number.

I_1^α possesses both coagulation and fragmentation coefficients. It is natural to assume the coagulation coefficients $a_{\alpha,\beta}^{j,k}$ scale in a similar way to the elastic collision coefficients, i.e. they are proportional to $c r_1^2$. By consistency we then assume the fragmentation coefficients $b_{\alpha+1}^j$ are proportional to $c r_1^2 \mathcal{R}$.

Thus setting

$$\begin{aligned} a_{\alpha,1}^{j,k} &= c r_1^2 \bar{a}_{\alpha,1}^{j,k} \frac{\varepsilon}{\mu} \\ b_{\alpha+1}^j &= c r_1^2 \mathcal{R} \bar{b}_{\alpha+1}^j \frac{\varepsilon}{\mu} \end{aligned}$$

where μ is the dimensionless inelastic Knudsen number, and $\bar{I}_1^\alpha$ is I_1^α with n_j^α replaced by $\bar{n}_j^\alpha$, $a_{\alpha,1}^{j,k}$, $b_{\alpha+1}^j$ replaced by the above definitions, we see

$$\frac{\partial \bar{n}_1^\alpha}{\partial \bar{t}} + \frac{1}{\alpha}\frac{\partial \bar{n}_1^\alpha}{\partial \bar{x}} = \frac{\bar{E}_1^\alpha}{\varepsilon} + \frac{\bar{I}_1^\alpha}{\mu}.$$

Finally drop the over bars and we have derived system

$$\begin{aligned}
\frac{\partial n_1^\alpha}{\partial t} + \frac{1}{\alpha}\frac{\partial n_1^\alpha}{\partial x} &= \frac{E_1^\alpha}{\varepsilon} + \frac{I_1^\alpha}{\mu}, \quad (a)\\
\frac{\partial n_2^\alpha}{\partial t} - \frac{1}{\alpha}\frac{\partial n_2^\alpha}{\partial x} &= \frac{E_2^\alpha}{\varepsilon} + \frac{I_2^\alpha}{\mu}, \quad (b)\\
\frac{\partial n_3^\alpha}{\partial t} + \frac{1}{\alpha}\frac{\partial n_3^\alpha}{\partial y} &= \frac{E_3^\alpha}{\varepsilon} + \frac{I_3^\alpha}{\mu}, \quad (c)\\
\frac{\partial n_4^\alpha}{\partial t} - \frac{1}{\alpha}\frac{\partial n_4^\alpha}{\partial y} &= \frac{E_4^\alpha}{\varepsilon} + \frac{I_4^\alpha}{\mu}, \quad (d) \qquad 1 \le \alpha \le M \\
\frac{\partial n_5^\alpha}{\partial t} + \frac{1}{\alpha}\frac{\partial n_5^\alpha}{\partial z} &= \frac{E_5^\alpha}{\varepsilon} + \frac{I_5^\alpha}{\mu}, \quad (e)\\
\frac{\partial n_6^\alpha}{\partial t} - \frac{1}{\alpha}\frac{\partial n_6^\alpha}{\partial z} &= \frac{E_6^\alpha}{\varepsilon} + \frac{I_6^\alpha}{\mu}, \quad (f)\\
\frac{\partial n_0^\alpha}{\partial t} &= \frac{I_0^\alpha}{\mu}. \quad (g)
\end{aligned} \tag{2.2}$$

We note that since in our model the total number of particles is always conserved, a cube of volume L^3 will have $\mathcal{R} = M_0/L^3$ where M_0 is the number of particles at $t = 0$. Of course M_0 must be less than or equal to M. Hence we have $\varepsilon = L^2/r_1^2 M_0$. In the Boltzmann limit [1] for rarefied gases we take $M_0 \to \infty$, $\left(\frac{r_1}{L}\right) \to 0$, $\mathrm{vol}(V) \to \infty$ with $\left(\frac{r_1}{L}\right)^2 M_0$ finite. This motivates our study of the case of $M = \infty$, ε finite. However in the Boltzmann limit for dense gases we take $M_0 \to \infty$, $\left(\frac{r_1}{L}\right) \to 0$, with $\left(\frac{r_1}{L}\right)^3 M_0$ finite i.e. since

$$\varepsilon = \frac{r_1 L^{-1}}{(r_1/L)^3 M_0},$$

we consider $\varepsilon \to 0$, the fluid dynamical limit.

Next record in addition the equations for transport of α-clusters

$$
\begin{aligned}
\tfrac{\partial}{\partial t}(N^\alpha) \;+\; \tfrac{\partial}{\partial x}(N^\alpha u^\alpha) \;+\; \tfrac{\partial}{\partial y}(N^\alpha v^\alpha)& \\
+\; \tfrac{\partial}{\partial z}(N^\alpha w^\alpha) \;=\; \tfrac{J_{\alpha-1}-J_\alpha}{\mu}\,, \quad 2 \le \alpha \le M&
\end{aligned}
\tag{2.3}
$$

$$
\begin{aligned}
\tfrac{\partial}{\partial t}N^1 \;+\; \tfrac{\partial}{\partial x}(N^1 u^1) \;+\; \tfrac{\partial}{\partial y}(N^1 v^1)& \\
+\; \tfrac{\partial}{\partial z}(N^1 w^1) \;=\; \tfrac{-J_1-\sum_{\alpha=1}^{M} J_\alpha}{\mu}&
\end{aligned}
\tag{2.4}
$$

where

$$
\begin{aligned}
N^\alpha &\doteq \sum_{j=0}^{6} n_j^\alpha \,, \\
N^\alpha u^\alpha &\doteq \frac{1}{\alpha}(n_1^\alpha - n_2^\alpha) \,, \\
N^\alpha v^\alpha &\doteq \frac{1}{\alpha}(n_3^\alpha - n_4^\alpha) \,, \\
N^\alpha w^\alpha &\doteq \frac{1}{\alpha}(n_5^\alpha - n_6^\alpha) \,;
\end{aligned}
$$

the equation for conservation of mass

$$
\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0 \,, \tag{2.5}
$$

where

$$
\begin{aligned}
\rho &\doteq \sum_{\alpha=1}^{M} \alpha N^\alpha \,, \\
\rho u &\doteq \sum_{\alpha=1}^{M} \alpha N^\alpha u^\alpha = \sum_{\alpha=1}^{M} (n_1^\alpha - n_2^\alpha) \,, \\
\rho v &\doteq \sum_{\alpha=1}^{M} \alpha N^\alpha v^\alpha = \sum_{\alpha=1}^{M} (n_3^\alpha - n_4^\alpha) \,, \\
\rho w &\doteq \sum_{\alpha=1}^{M} \alpha N^\alpha w^\alpha = \sum_{\alpha=1}^{M} (n_5^\alpha - n_6^\alpha) \,;
\end{aligned}
$$

and the equation for conservation of linear momentum

$$
\begin{aligned}
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\sum_{\alpha=1}^{M}\frac{1}{\alpha}(n_1^\alpha + n_2^\alpha) &= 0\,, \\
\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial y}\sum_{\alpha=1}^{M}\frac{1}{\alpha}(n_3^\alpha + n_4^\alpha) &= 0\,, \\
\frac{\partial}{\partial t}(\rho w) + \frac{\partial}{\partial z}\sum_{\alpha=1}^{M}\frac{1}{\alpha}(n_5^\alpha + n_6^\alpha) &= 0\,.
\end{aligned}
\tag{2.6}
$$

If we define the macroscopic symmetric tensor Π by

$$
\begin{aligned}
\Pi_{xx} &= -\rho u^2 + \sum \frac{1}{\alpha}(n_1^\alpha + n_2^\alpha)\,, \\
\Pi_{yy} &= -\rho v^2 + \sum \frac{1}{\alpha}(n_3^\alpha + n_4^\alpha)\,, \\
\Pi_{zz} &= -\rho w^2 + \sum \frac{1}{\alpha}(n_5^\alpha + n_6^\alpha)\,, \\
\Pi_{xy} &= -\rho uv,\ \Pi_{xz} = -\rho uw,\ \Pi_{yz} = -\rho vw
\end{aligned}
$$

then the conservation of linear momentum may be expressed in the familiar form

$$
\begin{aligned}
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) + \frac{\partial}{\partial y}(\rho uv) + \frac{\partial}{\partial z}(\rho uw) + \frac{\partial}{\partial x}\Pi_{xx} + \frac{\partial}{\partial y}\Pi_{xy} + \frac{\partial}{\partial z}\Pi_{xz} &= 0\,, \\
\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho vu) + \frac{\partial}{\partial x}(\rho v^2) + \frac{\partial}{\partial z}(\rho vw) + \frac{\partial}{\partial x}\Pi_{yx} + \frac{\partial}{\partial y}\Pi_{yy} + \frac{\partial}{\partial z}\Pi_{yz} &= 0\,, \\
\frac{\partial}{\partial t}(\rho w) + \frac{\partial}{\partial x}(\rho wu) + \frac{\partial}{\partial y}(\rho wv) + \frac{\partial}{\partial z}(\rho w^2) + \frac{\partial}{\partial x}\Pi_{zx} + \frac{\partial}{\partial y}\Pi_{zy} + \frac{\partial}{\partial z}\Pi_{zz} &= 0\,.
\end{aligned}
\tag{2.7}
$$

In this paper, we consider only the two space dimensions by setting $n_j^\alpha(x,y,z,t) = n_j^\alpha(x,y,t)$, making the symmetry assumption $n_5^\alpha(x,y,t) = n_6^\alpha(x,y,t)$ and forcing $w \equiv 0$. As noted above in the Boltzmann limit we take $M = \infty$.

§3 A simple scaling analysis

Consider the transport equation (2.2) in the Boltzmann limit $M = \infty$. We wish to study the behavior in the neighborhood of wall $x = 0$. First we rescale x, t and set $\hat{x} = \frac{x}{\epsilon}$, $\hat{t} = \frac{t}{T}$

where T is a typical dimensionless time. Substitution of this scaling into (2.2a) yields for example

$$\frac{1}{T}\frac{\partial n_1^\alpha}{\partial \hat{t}} + \frac{1}{\varepsilon\alpha}\frac{\partial n_1^\alpha}{\partial \hat{x}} = \frac{E_1^\alpha}{\varepsilon} + \frac{I_1^\alpha}{\mu} .$$

Hence for small time when $T = \varepsilon$ we find to leading order the system is governed by the elastic collision system

$$\begin{aligned}
\frac{\partial n_1^\alpha}{\partial \hat{t}} + \frac{1}{\alpha}\frac{\partial n_1^\alpha}{\partial \hat{x}} &= E_1^\alpha , \quad (a) \\
\frac{\partial n_2^\alpha}{\partial \hat{t}} - \frac{1}{\alpha}\frac{\partial n_2^\alpha}{\partial \hat{x}} &= E_2^\alpha , \quad (b) \\
\frac{\partial n_3^\alpha}{\partial \hat{t}} &= E_3^\alpha , \quad (c) \qquad 1 \le \alpha < \infty \\
\frac{\partial n_4^\alpha}{\partial \hat{t}} &= E_4^\alpha , \quad (d) \\
\frac{\partial n_5^\alpha}{\partial \hat{t}} &= E_5^\alpha , \quad (e) \\
\frac{\partial n_0^\alpha}{\partial \hat{t}} &= 0 , \quad (f)
\end{aligned} \tag{3.1}$$

as long as y is outside a layer of width ε from the $y = 0$ wall.

On the other hand for larger times when $\frac{\varepsilon}{T} << 1$ we recover the equations

$$\begin{aligned}
\frac{1}{\alpha}\frac{\partial n_1^\alpha}{\partial \hat{x}} &= E_1^\alpha , \quad (a) \\
-\frac{1}{\alpha}\frac{\partial n_2^\alpha}{\partial \hat{x}} &= E_2^\alpha , \quad (b) \\
\frac{\mu}{T}\frac{\partial n_0^\alpha}{\partial \hat{t}} &= I_0^\alpha , \quad (c)
\end{aligned} \tag{3.2}$$

$$0 = E_3^\alpha = E_4^\alpha = E_5^\alpha . \tag{3.3}$$

For intermediate time $T = \mu$, (3.2c) yields the dynamic equation

$$\frac{\partial n_6^\alpha}{\partial \hat{t}} = I_0^\alpha \quad (T = \mu) \tag{3.4}$$

while for large time (3.2c) $T >> \mu$ yields the constraint

$$0 = I_0^\alpha \quad (T >> \mu)\,. \tag{3.5}$$

In the neighborhood of the vertex $x = 0$, $y = 0$ we rescale y in a similar manner $\hat{y} = \frac{y}{\varepsilon}$, $T = \varepsilon$ yielding the system

$$\begin{aligned}
\frac{\partial n_1^\alpha}{\partial \hat{t}} + \frac{1}{\alpha}\frac{\partial n_1^\alpha}{\partial \hat{x}} &= E_1^\alpha\,, \quad (a)\\
\frac{\partial n_2^\alpha}{\partial \hat{t}} - \frac{1}{\alpha}\frac{\partial n_2^\alpha}{\partial \hat{x}} &= E_2^\alpha\,, \quad (b)\\
\frac{\partial n_3^\alpha}{\partial \hat{t}} + \frac{1}{\alpha}\frac{\partial n_3^\alpha}{\partial \hat{y}} &= E_3^\alpha\,, \quad (c) \qquad 1 \le \alpha < \infty\\
\frac{\partial n_4^\alpha}{\partial \hat{t}} - \frac{1}{\alpha}\frac{\partial n_4^\alpha}{\partial \hat{y}} &= E_4^\alpha\,, \quad (d)\\
\frac{\partial n_5^\alpha}{\partial \hat{t}} &= E_5^\alpha\,, \quad (e)\\
\frac{\partial n_0^\alpha}{\partial \hat{t}} &= 0\,, \quad (f)
\end{aligned} \tag{3.6}$$

Again for larger times $\frac{\varepsilon}{T} << 1$ we recover the equations

$$\begin{aligned}
\frac{1}{\alpha}\frac{\partial n_1^\alpha}{\partial \hat{x}} &= E_1^\alpha\,, \quad (a)\\
-\frac{1}{\alpha}\frac{\partial n_2^\alpha}{\partial \hat{x}} &= E_2^\alpha\,, \quad (b)\\
\frac{1}{\alpha}\frac{\partial n_3^\alpha}{\partial \hat{y}} &= E_3^\alpha\,, \quad (c) \qquad 1 \le \alpha < \infty\\
-\frac{1}{\alpha}\frac{\partial n_4^\alpha}{\partial \hat{y}} &= E_4^\alpha\,, \quad (d)\\
0 &= E_5^\alpha\,, \quad (e)\\
\frac{\mu}{T}\frac{\partial n_0^\alpha}{\partial \hat{t}} &= I_0^\alpha\,. \quad (f)
\end{aligned} \tag{3.7}$$

Again for $T = \mu$ and $T >> \mu$ we obtain (3.4), (3.5) respectively from (3.7f).

Notice of course for y independent motion (3.7) reduces to (3.2), (3.3). Thus for large time $T >> \mu$, the motion in an $\varepsilon-$neighborhood of the wall $x = 0$ for one dimensional flow

and in a square with sides of length ε near $x = 0$, $y = 0$ for two dimensional flow is governed by steady elastic collisions combined with the constraint $I_0^\alpha = 0$.

Now we must do the analysis on the larger μ scale. The crucial step is to rewrite the cluster balance laws (2.3), (2.4) in the scaled variables $\hat{t} = \frac{t}{T}$, $x^* = \frac{x}{\mu}$, $y^* = \frac{y}{\mu}$. In this notation (2.3), (2.4) become

$$\frac{\mu}{T}\frac{\partial}{\partial \hat{t}}(N^\alpha) + \frac{\partial}{\partial x^*}(N^\alpha u^\alpha) + \frac{\partial}{\partial y^*}(N^\alpha v^\alpha) = J_{\alpha-1} - J_\alpha\,, \qquad 2 \le \alpha < \infty\,, \tag{3.8}$$

$$\frac{\mu}{T}\frac{\partial}{\partial \hat{t}}N^1 + \frac{\partial}{\partial x^*}(N^1 u^1) + \frac{\partial}{\partial y^*}(N^1 v^1) = -J_1 - \sum_{\alpha=1}^{\infty} J_\alpha\,. \tag{3.9}$$

On the same time scale $T = \varepsilon$ the elastic terms dominate and we find from (2.2) the spatially homogeneous system

$$\frac{\partial n_j^\alpha}{\partial \hat{t}} - E_j^\alpha = 0\,, \quad 1 \le j \le 6,\ 1 \le \alpha < \infty \tag{3.10}$$

$$\frac{\partial n_0^\alpha}{\partial \hat{t}} = 0\,, \quad 1 \le \alpha < \infty\,. \tag{3.11}$$

On the intermediate scale $T = \mu$ spatially inhomogeneities enter via (3.8), (3.9) and we obtain the equations

$$\frac{\partial}{\partial \hat{t}}(N^\alpha) + \frac{\partial}{\partial x^*}(N^\alpha u^\alpha) + \frac{\partial}{\partial y^*}(N^\alpha v^\alpha) = J_{\alpha-1} - J_\alpha\,, \qquad 2 \le \alpha < \infty \tag{3.12}$$

$$\frac{\partial}{\partial \hat{t}}N^1 + \frac{\partial}{\partial x^*}(N^1 u^1) + \frac{\partial}{\partial y^*}(N^1 v^1) = -J_1 - \sum_{\alpha=1}^{\infty} J_\alpha\,, \tag{3.13}$$

combined with

$$\frac{\partial n_0^\alpha}{\partial \hat{t}} = I_0^\alpha \tag{3.14}$$

from (2.2g). In addition we have the constraint that the solution evolve on an elastic Maxwellian

$$E_j^\alpha = 0\,, \quad 1 \le j \le 6,\ 1 \le \alpha < \infty\,, \tag{3.15}$$

from (2.2a-e).

We recall from [8] that (3.15) implies

$$(n_1^\alpha, n_2^\alpha, n_3^\alpha, n_4^\alpha, n_5^\alpha) = (e^{c_1}, e^{-c_1}, e^{c_2}, e^{-c_2}, 1)C^\alpha \ , \quad \alpha = 1, \cdots . \tag{3.16}$$

For longer times $T >> \mu$ (3.12), (3.13), (3.14) reduce to their time independent steady state versions obtained by setting time derivatives equal to zero.

For motions where $x >> \mu$, $y >> \mu$, $t >> \mu$ the fluid dynamic limit becomes the dominant system:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) &= 0 \, . \\ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\sum_{\alpha=1}^{\infty}\frac{1}{\alpha}(n_1^\alpha + n_2^\alpha) &= 0 \, , \\ \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial y}\sum_{\alpha=1}^{\infty}\frac{1}{\alpha}(n_3^\alpha + n_4^\alpha) &= 0 \, , \end{aligned} \tag{3.17}$$

where n_j^α evolve along the manifold of elastic–inelastic Maxwellians (again see [8])

$$E_j^\alpha = I_j^\alpha = 0 \ , \quad 0 \leq j \leq 6 \ , \ 1 \leq \alpha < \infty \ ,$$

given by

$$\begin{aligned} (n_0^\alpha, n_1^\alpha, n_2^\alpha, n_3^\alpha, n_4^\alpha, n_5^\alpha) &= (1, e^{c_1}, e^{-c_1}, e^{c_2}, e^{-c_2}, 1)Q_\alpha (n_0^1)^\alpha \ , \\ Q_\alpha &= 2^{\alpha-2}\frac{a_{\alpha-1}\cdots a_1}{b_\alpha \cdots b_2} \ , \quad \alpha \geq 2 \\ Q_1 &= 1 \ , \end{aligned} \tag{3.18}$$

c_1, c_2, n_0^1 are functions of (x, y, t). In this case (3.17) yields a system of three conservation laws in the dependent variables $c_1(x,y,t)$, $c_2(x,y,t)$, $n_0^1(x,y,t)$. The system is meaningful in fluid dynamic limit $\varepsilon \to 0$ for finite values of the density ρ, i.e. when $0 \leq n_0^1 \leq z_s$ and z_s

is the radius of convergence for the power series

$$\sum_{\alpha=1}^{\infty} \alpha Q_\alpha z^\alpha .$$

Here $\rho_s = \sum_{\alpha=1}^{\infty} \alpha Q_\alpha z_s^\alpha$ is the saturation density.

Thus we conclude:

1. In an $\varepsilon-$layer near the wall the elastic Boltzmann like regime dominates given the (3.1)-(3.7).

2. In a wider layer of width μ the cluster transport is taking place. This layer interpolates between the macroscopic fluid equations (3.17) and the microscopic elastic collision Boltzmann like dynamics (3.1)-(3.7). This wider μ layer is governed by equations (3.8)-(3.16).

There is one additional scaling that is appealing to make in the transition layer of width μ, $T = \mu$ when (3.12)-(3.16) are valid. Specifically we follow the discussion of Zel'dovich and Raizer [10, VI, Section 18] and treat α as a continuous variable, $1 \leq \alpha < \infty$. This yields the rule for evolution along elastic Maxwellians as

$$(n_1(x,y,\alpha,t), n_2(x,y,\alpha,t), n_3(x,y,\alpha,t), n_4(x,y,\alpha,t), n_5)(x,y,\alpha,t)$$
$$= (e^{c_1}, e^{-c_1}, e^{c_2}, e^{-c_2}, 1)C(x,y,\alpha,t)\,, \quad 1 \leq \alpha < \infty\,, \tag{3.19}$$

where c_1, c_2 are functions of (x,y,t). Then we find

$$\begin{aligned} N(x,y,\alpha,t) &= \sum_{j=0}^{6} n_j(x,y,\alpha,t) \\ &= n_0(x,y,\alpha,t) \\ &\quad + C(x,y,\alpha,t)(2\cosh c_1 + 2\cosh c_2 + 2)\,, \end{aligned} \tag{3.20}$$

$$N(x,y,\alpha,t)u(x,y,\alpha,t) = \frac{2}{\alpha}(\sinh(c_1(x,y,t))C(x,y,\alpha,t)\,, \tag{3.21}$$

$$N(x,y,\alpha,t)v(x,y,\alpha,t) = \frac{2}{\alpha}(\sinh(c_2(x,y,t))C(x,y,\alpha,t)\,, \tag{3.22}$$

$$\begin{aligned} J(x,y,\alpha,t) = {} & a(\alpha)n_0(x,y,\alpha,t)C(x,y,\alpha,t)(2\cosh c_1 + 2\cosh c_2 + 2) \\ & + a(\alpha)n_0(x,y,1,t)C(x,y,\alpha,t)(2\cosh c_1 + 2\cosh c_2 + 2) \\ & + 3a(\alpha)C(x,y,1,t)C(x,y,\alpha,t) \\ & + 3a(\alpha)C(x,y,1,t)C(x,y,\alpha,t) \\ & - b(\alpha)C(x,y,\alpha,t)(2\cosh c_1 + 2\cosh c_2 + 2) \\ & - (2\cosh c_1 + 2\cosh c_2 + 2)\frac{\partial}{\partial\alpha}(b(\alpha)C(x,y,\alpha.t))\,, \end{aligned} \tag{3.23}$$

$$\begin{aligned} I_0(x,y,\alpha,t) = {} & 3b(\alpha)n_0(x,y,\alpha,t) + 3a(\alpha)C(x,y,1,t)C(x,y,\alpha,t) \\ & -3C(x,y,1,t)\frac{\partial}{\partial\alpha}(a(\alpha)C(x,y,\alpha,t)) \\ & +3a(\alpha)C(x,y,1,t)C(x,y,\alpha,t) \\ & -3C(x,y,1,t)\frac{\partial}{\partial\alpha}(a(\alpha)C(x,y,\alpha,t)) \\ & -a(\alpha)C(x,y,1,t)C(x,y,\alpha,t)(2\cosh c_1 + 2\cosh c_2 + 2) \\ & -\frac{1}{2}b(\alpha)C(x,y,\alpha,t)(2\cosh c_1 + 2\cosh c_2 + 2) \\ & -\frac{1}{2}(2\cosh c_1 + 2\cosh c_2 + 2)\frac{\partial}{\partial\alpha}(b(\alpha)C(x,y,\alpha,t))\,,\ \alpha >> 1\,, \end{aligned} \tag{3.24}$$

$$\begin{aligned} I_0(x,y,1,t) = {} & -\int_{\beta=1}^{\infty} a(\beta)n_0(x,y,1,t)C(x,y,\beta,t)(2\cosh c_1 + 2\cosh c_2 + 2) \\ & -\frac{1}{2}\left\{b(\beta)C(x,y,\beta,t)(2\cosh c_1 + 2\cosh c_2 + 2)\right. \\ & \left. +\frac{\partial}{\partial\beta}\left[b(\beta)C(x,y,\beta,t)(2\cosh c_1 + 2\cosh c_2 + 2)\right]\right\} d\beta\,. \end{aligned}$$

Here we have conveniently though not rigorously regarded 1 as a small parameter when

$\alpha >> 1$ and used the approximation

$$f(\alpha+1) \approx f(\alpha) + f'(\alpha) \, .$$

If we combine (3.23) (3.24) with the continuous version of (3.12) we find for large α that the governing equations become the conservation laws

$$\begin{aligned} \frac{\partial}{\partial \hat{t}}(N) + \frac{\partial}{\partial x^*}(Nu) + \frac{\partial}{\partial y^*}(Nv) + \frac{\partial J}{\partial \alpha} &= 0 \qquad (3.25) \\ \frac{\partial}{\partial \hat{t}} n_0(x,y,\alpha,t) &= I_0(x,y,\alpha,t) \qquad (3.26) \end{aligned}$$

where N, Nu, Nv, J, I_0 are given by (3.20)-(3.24). This provides a system of equations for the variables $n_0^*(x^*,y^*,\alpha.\hat{t})$, $C^*(x^*,y^*,\alpha,\hat{t})$, $c_1^*(x^*,y^*,\hat{t})$, $c_2^*(x^*,y^*,\hat{t})$ obtained from n_0, C, c_1, c_2 by the indicated change of variables. When combined with the equations of conservation of momentum (2.6a,b) written along (3.19) we have four equations in four unknowns depending on the four independent variables x^*, y^*, α, $\hat{t}$. Unfortunately (3.25), (3.26) will possess the nonlocal "boundary" terms $C(x,y,1,t)$ $n_0(x,y,1,t)$ which must be obtained from the continuous versions of (3.13), (3.14):

$$\begin{aligned} \frac{\partial}{\partial \hat{t}} N(x,y,1,t) \;&+\; \frac{\partial}{\partial x^*}(N(x,y,1,t)u(x,y,1,t)) \;+\; \frac{\partial}{\partial y^*}(N(x,y,1,t)v(x,y,1,t)) \\ &= \; -J(x,y,1,t) - \int_1^\infty J(x,y,\alpha,t)d\alpha \, , \qquad (3.27) \\ \frac{\partial}{\partial \hat{t}} n_0(x,y,1,t) \;&=\; I_0(x,y,1,t) \, . \qquad (3.28) \end{aligned}$$

A continuous approximation of (3.12) would envolve solving (2.5), (2.6) (subject to (3.19)), (3.25), (3.26) for $\alpha > 1$ with boundary conditions (3.27), (3.28) and appropriate initial conditions for n_0^*, C^*, c_1^*, c_2^*.

§4 Numerical simulations

In this section, we present the numerical simulations of a gas impinging upon wall(s) in a two dimensional square box. We assume specularly reflecting boundary conditions. Using the discrete velocity model, we expect to observe the nucleation, that is the formation of larger clusters, on the boundary where the gas impinges.

The numerical implementation of the model is straight forward except for the method used to solve the partial differential equations (2.2). For that we used the first order upwind scheme to discretize (2.2). Also we require the closure hypothesis $J_M = 0$ to enforce mass conservation, M finite. The calculations are carried out at U-W Madison on an HP710 provided by NSF under a SCREMS grant. The color pictures were created on an SGI machine.

The kinetic coefficients in the inelastic collision process are computed with the formulas used by Penrose, Lebowitz, Marro, Kalos, and Tobochnik [6]:

$$2a_\alpha = \frac{1}{6}(874 + 1888\alpha)^{1/3}\ , \quad 2 \leq \alpha < \infty\ , \tag{4.1}$$

$$b_{\alpha+1} = 2w_\alpha a_\alpha\ ,\ 2 \leq \alpha\ , \tag{4.2}$$

$$w_\alpha = \frac{Q_\alpha}{Q_{\alpha+1}} = w_s\Big[1 + \frac{2.415}{(\alpha-2)^{1/3}}\Big]\ ,\ 3 \leq \alpha < \infty \tag{4.3}$$

$$w_s = 0.010526\ . \tag{4.4}$$

For the case $\alpha = 1$

$$a_1 = \frac{1}{6}(874 + 1888)^{1/3} \tag{4.5}$$

and

$$w_\alpha = \frac{Q_\alpha}{Q_{\alpha+1}}\ ,\ \alpha = 1, 2\ . \tag{4.6}$$

$$b_3 = 2w_2 a_2 \ , \ b_2 = w_1 a_1 \ . \tag{4.7}$$

$Q_1 = 1$ and we choose $Q_2 = \exp(2.599)$, $Q_3 = \exp(5.708)$ from the equilibrium simulation of Stauffer, Coniglio, and Heerman [9] given in Table 1 of [6].

The initial data are given by the formulas

$$(n_0^\alpha, n_1^\alpha, n_2^\alpha, n_3^\alpha, n_4^\alpha, n_5^\alpha) \ = \ (0,0,0,0,0) \ , \ 2 \leq \alpha < M \tag{4.8}$$

$$(n_0^1, n_1^1, n_2^1, n_3^1, n_4^1, n_5^1) \ = \ (1, e^{c_1}, e^{-c_1}, e^{c_2}, e^{-c_2}, 1) Q_1 n_0^1 \ , \tag{4.9}$$

Therefore initially, we have only the 1-clusters in the system.

Choosing $n_0^1 = 1.0$, $c_1 = 2.0$, $c_2 = 0.0$, Knudsen numbers $\varepsilon = 15$ and $\mu = 30$ and $M = 8$, we have a case that can be reduced to one dimensional model. The Fig. 1(a)(b)(c)(d) are illustrated the density distribution of the gas at time steps 50, 150, 250 and 350 respectively. In all of gray scale photo pictures, the variations of gray scale from white to grey to black correspond to the density variations from zero density to lower density to highest density. The gas impinged upon one side wall and was drawn off from the opposite wall. The Fig. 2(a)(b)(c)(d) shows the density distribution of total nucleated clusters, that is the all clusters except of the 1-clusters, for the corresponding steps as in the Fig. 1(a)(b)(c)(d). The nucleation process are clearly visible and proportional to the density distribution of the gas at the side of impinged wall.

The Fig. 3(a)(b)(c)(d) show the density distribution at steps 50, 150, 250 and 350 respectively for the gas sending to a corner of the square box. Here $n_0^1 = 1.0$, $c_1 = 2.0$, $c_2 = 2.0$. $\varepsilon = 20$, $\mu = 40$ and $M = 8$. The Fig. 4(a)(b)(c)(d) show the corresponding nucleation density distributions. The Fig 3 and 4 are illustrated the similar phenomenon as in the Fig 1 and 2 except that in the Fig 3 and 4, the phenomenon is not reducible to one

dimensional model. Both computational visualizations show the formation of two layers, one nested within the other at the boundary.

§5 Conclusion

We have performed a numerical simulation for the discrete velocity kinetic model with coagulation and fragmentation originally described in [8]. The computations illustrate the formation of a boundary layer containing the large clusters (denser vapor) which is contained within a thicker layer in which the rarefied vapor is being converted to the denser vapor. Of course the computations only reflect the two length scales built into the original model: ε, μ. In an $\varepsilon-$neighborhood of the wall the elastic collisions dominate and coagulation and fragmentation ceases while on a larger $\mu-$neighborhood and away from the wall it is the inelastic collisions with the flow evolving along the manifold of elastic Maxwellians which dominate. Since it is the inelastic collisions that cause the nucleation we observe nucleation occurring through the wider $\mu-$layer. Outside the wider μ layer the macroscopic conservation laws of mass and momentum (isothermal, compressible Euler equations) are valid. This is meaningful in the infinite limit $M \to \infty$ as long as $0 \leq \rho \leq \rho_s$, ρ_s the saturation density. In the μ, ε layers we have no such restriction and ρ can exceed ρ_s.

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APPENDIX

Formulas for elastic terms E_j^α:

$$
\begin{aligned}
E_1^\alpha &= \frac{4}{3}\frac{\sigma_{\alpha\alpha}c}{\alpha}(n_3^\alpha n_4^\alpha + n_5^\alpha n_6^\alpha - 2n_1^\alpha n_2^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} \frac{c\sigma_{\alpha\beta}}{6}\Big(\frac{1}{\alpha}+\frac{1}{\beta}\Big)(n_1^\beta n_2^\alpha + n_3^\alpha n_4^\beta + n_3^\beta n_4^\alpha \\
&\qquad + n_5^\alpha n_6^\beta + n_5^\beta n_6^\alpha - 5n_1^\alpha n_2^\beta) \\
&+ \sum_{\beta\neq\alpha}^{M} c\sigma_{\alpha\beta}R_{\alpha\beta}(n_1^\beta n_3^\alpha + n_1^\beta n_4^\alpha + n_1^\beta n_5^\alpha + n_1^\beta n_6^\alpha \\
&\qquad - n_1^\alpha n_3^\beta - n_1^\alpha n_4^\beta - n_1^\alpha n_5^\beta - n_1^\alpha n_6^\beta)\ , \\
E_2^\alpha &= \frac{4}{3}\frac{\sigma_{\alpha\alpha}c}{\alpha}(n_3^\alpha n_4^\alpha + n_5^\alpha n_6^\alpha - 2n_1^\alpha n_2^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} \frac{c\sigma_{\alpha\beta}}{6}\Big(\frac{1}{\alpha}+\frac{1}{\beta}\Big)(n_1^\alpha n_2^\beta + n_3^\alpha n_4^\beta + n_3^\beta n_4^\alpha \\
&\qquad + n_5^\alpha n_6^\beta + n_5^\beta n_6^\alpha - 5n_2^\alpha n_1^\beta) \\
&+ \sum_{\beta\neq\alpha}^{M} c\sigma_{\alpha\beta}R_{\alpha\beta}(n_2^\beta n_3^\alpha + n_2^\beta n_4^\alpha + n_2^\beta n_5^\alpha + n_2^\beta n_6^\alpha \\
&\qquad - n_2^\alpha n_3^\beta - n_2^\alpha n_4^\beta - n_2^\alpha n_5^\beta - n_2^\alpha n_6^\beta)\ , \\
E_3^\alpha &= \frac{4}{3}\frac{\sigma_{\alpha\alpha}c}{\alpha}(n_1^\alpha n_2^\alpha + n_5^\alpha n_6^\alpha - 2n_3^\alpha n_4^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} \frac{c\sigma_{\alpha\beta}}{6}\Big(\frac{1}{\alpha}+\frac{1}{\beta}\Big)(n_3^\beta n_4^\alpha + n_1^\alpha n_2^\beta + n_1^\beta n_2^\alpha \\
&\qquad + n_5^\alpha n_6^\beta + n_5^\beta n_6^\alpha - 5n_3^\alpha n_4^\beta) \\
&+ \sum_{\beta\neq\alpha}^{M} c\sigma_{\alpha\beta}R_{\alpha\beta}(n_3^\beta n_1^\alpha + n_3^\beta n_2^\alpha + n_3^\beta n_5^\alpha + n_3^\beta n_6^\alpha \\
&\qquad - n_3^\alpha n_1^\beta - n_3^\alpha n_2^\beta - n_3^\alpha n_5^\beta - n_3^\alpha n_6^\beta)\ , \\
E_4^\alpha &= \frac{4}{3}\frac{\sigma_{\alpha\alpha}c}{\alpha}(n_1^\alpha n_2^\alpha + n_5^\alpha n_6^\alpha - 2n_3^\alpha n_4^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} \frac{c\sigma_{\alpha\beta}}{6}\Big(\frac{1}{\alpha}+\frac{1}{\beta}\Big)(n_3^\alpha n_4^\beta + n_1^\alpha n_2^\beta + n_1^\beta n_2^\alpha \\
&\qquad + n_5^\alpha n_6^\alpha + n_5^\beta n_6^\alpha - 5n_3^\beta n_4^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} c\sigma_{\alpha\beta}R_{\alpha\beta}(n_4^\beta n_1^\alpha + n_4^\beta n_2^\alpha + n_4^\beta n_5^\alpha + n_4^\beta n_6^\alpha
\end{aligned}
$$

$$
\begin{aligned}
& -n_4^\alpha n_1^\beta - n_4^\alpha n_2^\beta - n_4^\alpha n_5^\beta - n_4^\alpha n_6^\beta) , \\
E_5^\alpha &= \frac{4}{3}\frac{\sigma_{\alpha\alpha}c}{\alpha}(n_1^\alpha n_2^\alpha + n_3^\alpha n_4^\alpha - 2n_5^\alpha n_6^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} \frac{c\sigma_{\alpha\beta}}{6}\Big(\frac{1}{\alpha}+\frac{1}{\beta}\Big)(n_5^\beta n_6^\alpha + n_1^\alpha n_2^\beta + n_1^\beta n_2^\alpha \\
&\quad + n_3^\alpha n_4^\beta + n_3^\beta n_4^\alpha - 5n_5^\alpha n_6^\beta) \\
&+ \sum_{\beta\neq\alpha}^{M} c\sigma_{\alpha\beta}R_{\alpha\beta}(n_5^\beta n_1^\alpha + n_5^\beta n_2^\alpha + n_5^\beta n_3^\alpha + n_5^\beta n_4^\alpha \\
&\quad - n_5^\alpha n_1^\beta - n_5^\alpha n_2^\beta - n_5^\alpha n_3^\beta - n_5^\alpha n_4^\beta) , \\
E_6^\alpha &= \frac{4}{3}\frac{\sigma_{\alpha\alpha}c}{\alpha}(n_1^\alpha n_2^\alpha + n_3^\alpha n_4^\alpha - 2n_5^\alpha n_6^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} \frac{c\sigma_{\alpha\beta}}{6}\Big(\frac{1}{\alpha}+\frac{1}{\beta}\Big)(n_5^\alpha n_6^\beta + n_1^\alpha n_2^\beta + n_1^\beta n_2^\alpha \\
&\quad + n_3^\alpha n_4^\beta + n_3^\beta n_4^\alpha - 5n_5^\beta n_6^\alpha) \\
&+ \sum_{\beta\neq\alpha}^{M} c\sigma_{\alpha\beta}R_{\alpha\beta}(n_6^\beta n_1^\alpha + n_6^\beta n_2^\alpha + n_6^\beta n_3^\alpha + n_6^\beta n_4^\alpha \\
&\quad - n_6^\alpha n_1^\beta - n_6^\alpha n_2^\beta - n_6^\alpha n_3^\beta - n_6^\alpha n_4^\beta) .
\end{aligned}
$$

Here $\sigma_{\alpha\beta}, cR_{\alpha\beta}$ denote the collisional cross sectional area and magnitude of relative velocities in a (n_j^α, n_k^β) collision. An estimate of $\sigma_{\alpha\beta}$ is easily obtained by noting that it is proportional to $(r_\alpha + r_\beta)^2$, r_α, r_β the radii of α- and β-clusters respectively. Since the volume of an α-cluster in $\frac{4}{3}\pi\alpha r_1^3$ the radius of a spherical α- cluster is $r_1\alpha^{1/3}$ and hence $\sigma_{\alpha\beta}$ is proportional to $r_1^2(\alpha^{1/3}+\beta^{1/3})^2$. To compute $R_{\alpha\beta}$ we note that the velocity of an n_j^α cluster is $\frac{p_j}{m\alpha}$ and an n_k^β cluster is $\frac{p_k}{m\beta}$. Hence $R_{\alpha\beta} = (\frac{1}{\alpha}+\frac{1}{\beta})$ for "head on" collisions and $R_{\alpha\beta} = (\frac{1}{\alpha^2}+\frac{1}{\beta^2})^{1/2}$ for collisions at a right angle.

Inelastic terms I_j^α for $2 \le \alpha \le M$:

$$
\begin{aligned}
I_1^\alpha &= a_{\alpha-1,1}^{0,1} n_1^1 n_0^{\alpha-1} + (1-\delta_{\alpha 2}) a_{\alpha-1,1}^{1,0} n_1^{\alpha-1} n_0^1 - b_\alpha^1 n_1^\alpha \\
&\quad + (1-\delta_{\alpha M})(-a_{\alpha,1}^{1,2} n_1^\alpha n_2^1 - a_{\alpha,1}^{1,0} n_1^\alpha n_0^1 + \frac{1}{2} b_{\alpha+1}^1 n_1^{\alpha+1} + \frac{1}{6} b_{\alpha+1}^0 n_0^{\alpha+1}) , \\
I_2^\alpha &= a_{\alpha-1,1}^{0,2} n_2^1 n_0^{\alpha-1} + (1-\delta_{\alpha 2}) a_{\alpha-1,1}^{2,0} n_2^{\alpha-1} n_0^1 - b_\alpha^2 n_2^\alpha
\end{aligned}
$$

$$+(1-\delta_{\alpha M})(-a^{2,1}_{\alpha,1}n^{\alpha}_2 n^1_1 - a^{2,0}_{\alpha,1}n^{\alpha}_2 n^1_0 + \frac{1}{2}b^2_{\alpha+1}n^{\alpha+1}_2 + \frac{1}{6}b^0_{\alpha+1}n^{\alpha+1}_0)\,,$$

$$\begin{aligned}
I^{\alpha}_3 &= a^{0,3}_{\alpha-1,1}n^1_3 n^{\alpha-1}_0 + (1-\delta_{\alpha 2})a^{3,0}_{\alpha-1,1}n^{\alpha-1}_3 n^1_0 - b^3_{\alpha}n^{\alpha}_3 \\
&\quad +(1-\delta_{\alpha M})(-a^{3,4}_{\alpha,1}n^{\alpha}_3 n^1_4 - a^{3,0}_{\alpha,1}n^{\alpha}_3 n^1_0 + \frac{1}{2}b^3_{\alpha+1}n^{\alpha+1}_3 + \frac{1}{6}b^0_{\alpha+1}n^{\alpha+1}_0)\,, \\
I^{\alpha}_4 &= a^{0,4}_{\alpha-1,1}n^1_4 n^{\alpha-1}_0 + (1-\delta_{\alpha 2})a^{4,0}_{\alpha-1,1}n^{\alpha-1}_4 n^1_0 - b^4_{\alpha}n^{\alpha}_4 \\
&\quad +(1-\delta_{\alpha M})(-a^{4,3}_{\alpha,1}n^{\alpha}_4 n^1_3 - a^{4,0}_{\alpha,1}n^{\alpha}_4 n^1_0 + \frac{1}{2}b^4_{\alpha+1}n^{\alpha+1}_4 + \frac{1}{6}b^0_{\alpha+1}n^{\alpha+1}_0)\,, \\
I^{\alpha}_5 &= a^{0,5}_{\alpha-1,1}n^1_5 n^{\alpha-1}_0 + (1-\delta_{\alpha 2})a^{5,0}_{\alpha-1,1}n^{\alpha-1}_5 n^1_0 - b^5_{\alpha}n^{\alpha}_5 \\
&\quad +(1-\delta_{\alpha M})(-a^{5,6}_{\alpha,1}n^{\alpha}_5 n^1_6 - a^{5,0}_{\alpha,1}n^{\alpha}_5 n^1_0 + \frac{1}{2}b^5_{\alpha+1}n^{\alpha+1}_5 + \frac{1}{6}b^0_{\alpha+1}n^{\alpha+1}_0)\,, \\
I^{\alpha}_6 &= a^{0,6}_{\alpha-1,1}n^1_6 n^{\alpha-1}_0 + (1-\delta_{\alpha 2})a^{6,0}_{\alpha-1,1}n^{\alpha-1}_6 n^1_0 - b^6_{\alpha}n^{\alpha}_6 \\
&\quad +(1-\delta_{\alpha M})(-a^{6,5}_{\alpha,1}n^{\alpha}_6 n^1_5 - a^{6,0}_{\alpha,1}n^{\alpha}_6 n^1_0 + \frac{1}{2}b^6_{\alpha+1}n^{\alpha+1}_6 + \frac{1}{6}b^0_{\alpha+1}n^{\alpha+1}_0)\,, \\
I^{\alpha}_0 &= -b^0_{\alpha}n^{\alpha}_0 + a^{2,1}_{\alpha-1,1}n^1_1 n^{\alpha-1}_2 + a^{4,3}_{\alpha-1,1}n^1_3 n^{\alpha-1}_4 + a^{6,5}_{\alpha-1,1}n^1_5 n^{\alpha-1}_6 \\
&\quad +(1-\delta_{\alpha 2})(a^{2,1}_{1,\alpha-1}n^{\alpha-1}_1 n^1_2 + a^{4,3}_{1,\alpha-1}n^{\alpha-1}_3 n^1_4 + a^{6,5}_{1,\alpha-1}n^{\alpha-1}_5 n^1_6) \\
&\quad +(1-\delta_{\alpha M})(-a^{0,1}_{\alpha,1}n^{\alpha}_0 n^1_1 - a^{0,2}_{\alpha,1}n^{\alpha}_0 n^1_2 - a^{0,3}_{\alpha,1}n^{\alpha}_0 n^1_3 \\
&\qquad -a^{0,4}_{\alpha,1}n^{\alpha}_0 n^1_4 - a^{0,5}_{\alpha,1}n^{\alpha}_0 n^1_5 - a^{0,6}_{\alpha,1}n^{\alpha}_0 n^1_6 + \frac{1}{2}b^1_{\alpha+1}n^{\alpha+1}_1 \\
&\quad +\frac{1}{2}b^2_{\alpha+1}n^{\alpha+1}_2 + \frac{1}{2}b^3_{\alpha+1}n^{\alpha+1}_3 + \frac{1}{2}b^4_{\alpha+1}n^{\alpha+1}_4 + \frac{1}{2}b^5_{\alpha+1}n^{\alpha+1}_5 \\
&\quad +\frac{1}{2}b^6_{\alpha+1}n^{\alpha+1}_6)\,.
\end{aligned}$$

Inelastic terms I^{α}_j for $\alpha = 1$:

$$\begin{aligned}
I^1_1 &= -\sum_{\beta=1}^{M-1}\left\{a^{1,2}_{1,\beta}n^1_1 n^{\beta}_2 + a^{1,0}_{1,\beta}n^1_1 n^{\beta}_0 - (1+\delta_{\beta 1})(\frac{1}{2}b^1_{1+\beta}n^{1+\beta}_1 + \frac{b^0_{1+\beta}}{6}n^{1+\beta}_0)\right\}, \\
I^1_2 &= -\sum_{\beta=1}^{M-1}\left\{a^{2,1}_{1,\beta}n^1_2 n^{\beta}_1 + a^{2,0}_{1,\beta}n^1_2 n^{\beta}_0 - (1+\delta_{\beta 1})(\frac{1}{2}b^2_{1+\beta}n^{1+\beta}_2 + \frac{b^0_{1+\beta}}{6}n^{1+\beta}_0)\right\}, \\
I^1_3 &= -\sum_{\beta=1}^{M-1}\left\{a^{3,4}_{1,\beta}n^1_3 n^{\beta}_4 + a^{3,0}_{1,\beta}n^1_3 n^{\beta}_0 - (1+\delta_{\beta 1})(\frac{1}{2}b^3_{1+\beta}n^{1+\beta}_3 + \frac{b^0_{1+\beta}}{6}n^{1+\beta}_0)\right\}, \\
I^1_4 &= -\sum_{\beta=1}^{M-1}\left\{a^{4,3}_{1,\beta}n^1_4 n^{\beta}_3 + a^{4,0}_{1,\beta}n^1_4 n^{\beta}_0 - (1+\delta_{\beta 1})(\frac{1}{2}b^4_{1+\beta}n^{1+\beta}_4 + \frac{b^0_{1+\beta}}{6}n^{1+\beta}_0)\right\},
\end{aligned}$$

$$I_5^1 = -\sum_{\beta=1}^{M-1}\left\{a_{1,\beta}^{5,6}n_5^1n_6^\beta + a_{1,\beta}^{5,0}n_5^1n_0^\beta - (1+\delta_{\beta 1})(\frac{1}{2}b_{1+\beta}^5 n_5^{1+\beta} + \frac{b_{1+\beta}^0}{6}n_0^{1+\beta})\right\},$$

$$I_6^1 = -\sum_{\beta=1}^{M-1}\left\{a_{1,\beta}^{6,5}n_6^1n_5^\beta + a_{1,\beta}^{6,0}n_6^1n_0^\beta - (1+\delta_{\beta 1})(\frac{1}{2}b_{1+\beta}^6 n_6^{1+\beta} + \frac{b_{1+\beta}^0}{6}n_0^{1+\beta})\right\},$$

$$\begin{aligned} I_0^1 = -\sum_{\beta=1}^{M-1}\Big\{ & a_{1,\beta}^{0,1}n_0^1n_1^\beta + a_{1,\beta}^{0,2}n_0^1n_2^\beta + a_{1,\beta}^{0,3}n_0^1n_3^\beta \\ & + a_{1,\beta}^{0,4}n_0^1n_4^\beta + a_{1,\beta}^{0,5}n_0^1n_5^\beta + a_{1,\beta}^{0,6}n_0^1n_6^\beta \\ & -\frac{1}{2}(1+\delta_{\beta 1})(b_{1+\beta}^1 n_1^{1+\beta} + b_{1+\beta}^2 n_2^{1+\beta} + b_{1+\beta}^3 n_3^{1+\beta} \\ & + b_{1+\beta}^4 n_4^{1+\beta} + b_{1+\beta}^5 n_5^{1+\beta} + b_{1+\beta}^6 n_6^{1+\beta})\Big\}. \end{aligned}$$

The $a_{\alpha,\beta}^{j,k}$ and $b_{\alpha+1}^j$ are positive kinetic rate coefficients for coagulation and fragmentation respectively. The $a_{\alpha,\beta}^{j,k}$ satisfy the principle of detailed balance $a_{\alpha,\beta}^{j,k} = a_{\beta,\alpha}^{j,k} = a_{\alpha,\beta}^{k,j}$. In general $a_{\alpha,\beta}^{j,k}$, $b_{\alpha+1}^j$ should depend on the volume V but in the classical Becker-Döring approach we use here they are assumed independent of V.

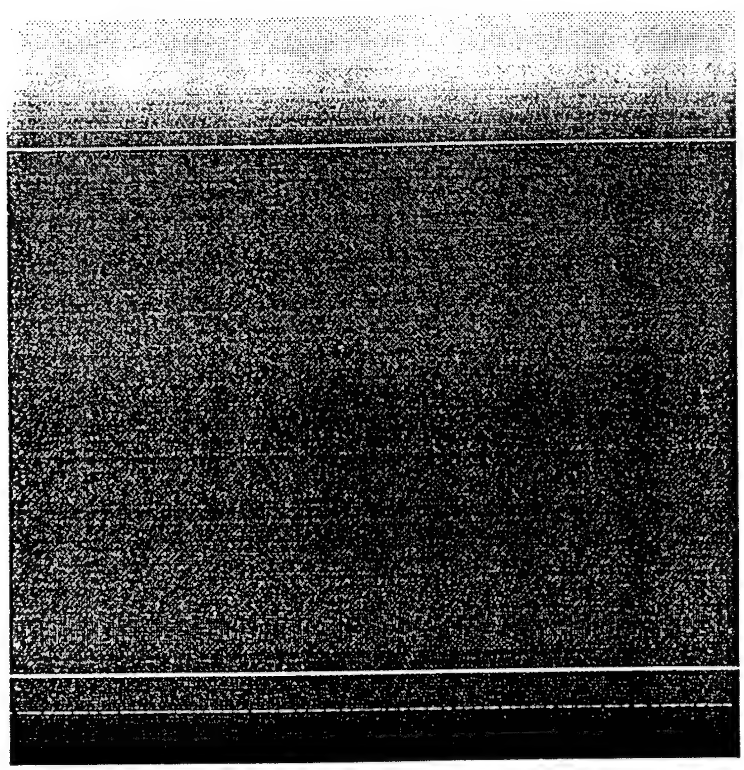

Fig 1(a) $t=50$

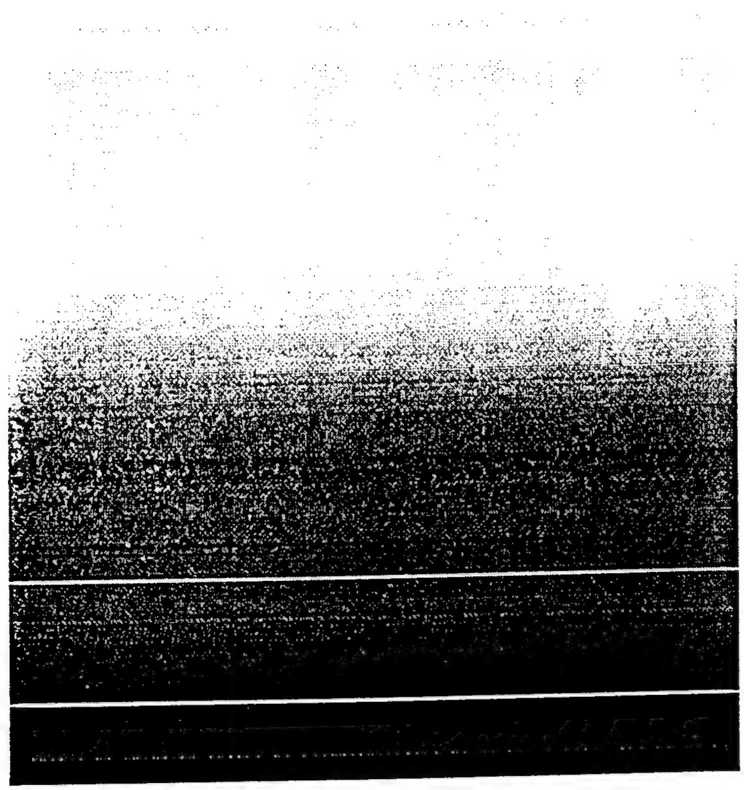

Fig 1(b) $t = 150$

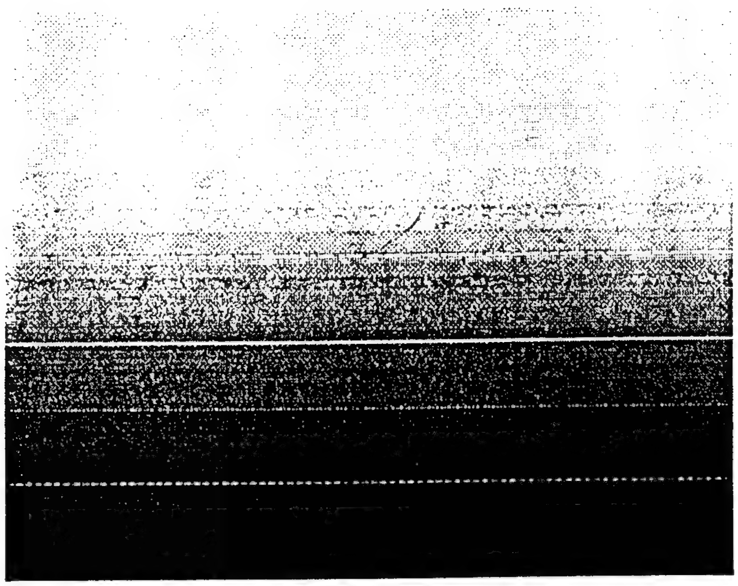

Fig 1 (c) $t=250$

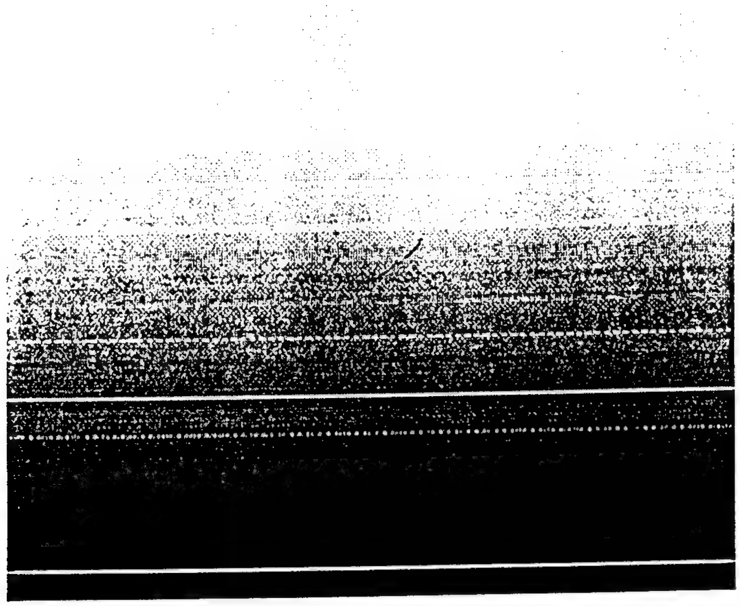

Fig 1 (d)   t = 350

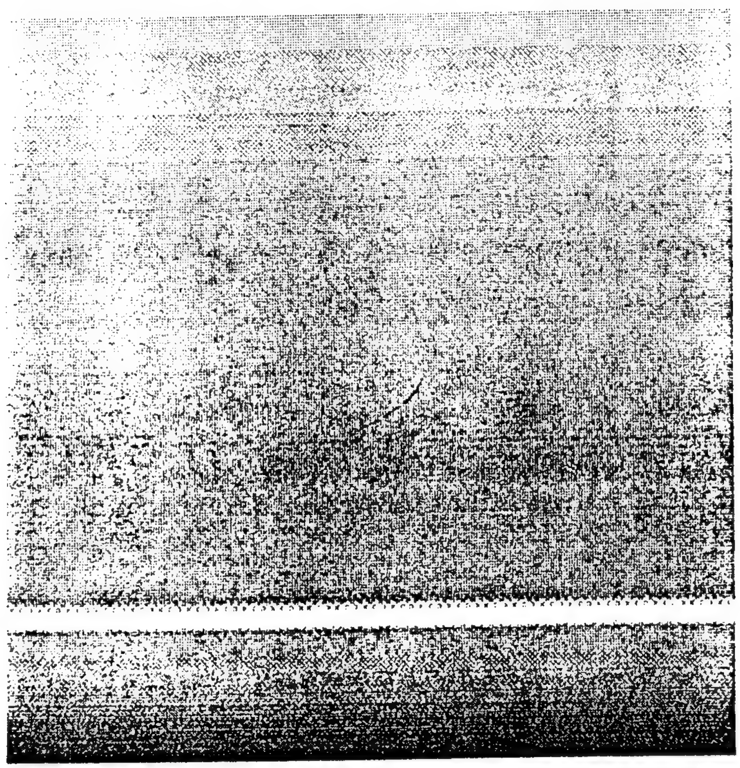

Fig 2 (a)   t=50

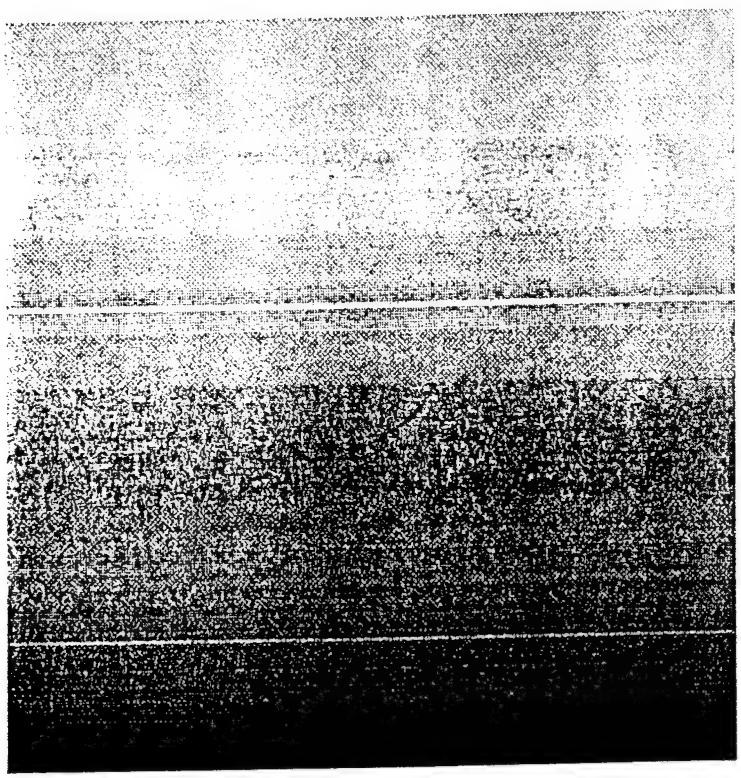

Fig 2 (b)   t=150

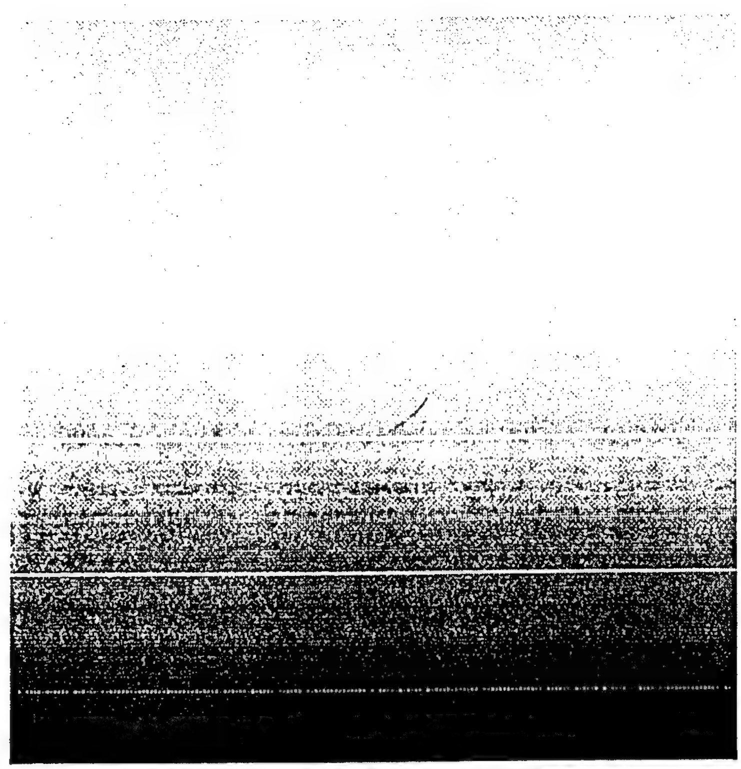

Fig 2 (c) $t=250$

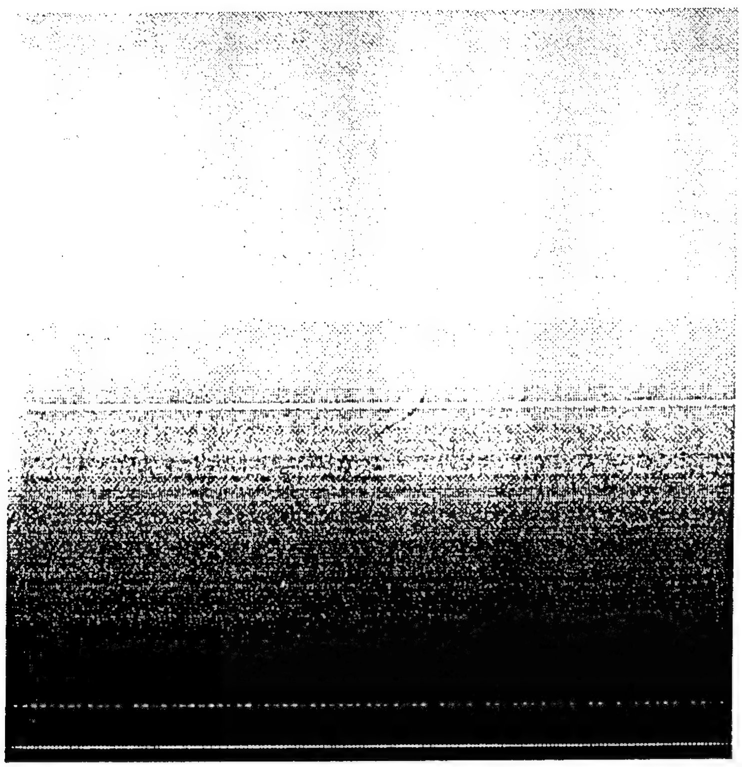

Fig 2(d) t=350

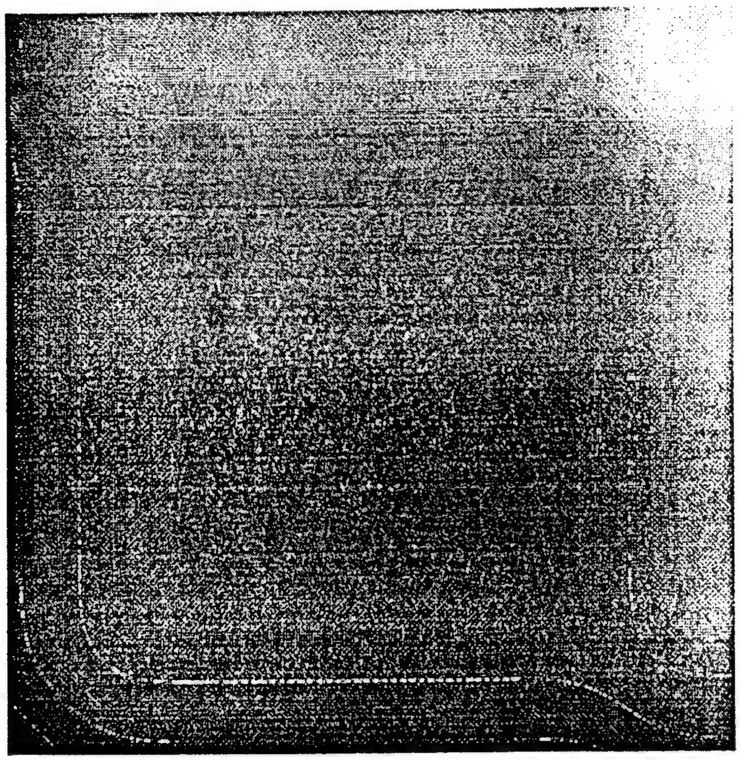

Fig 3 (a) t=50

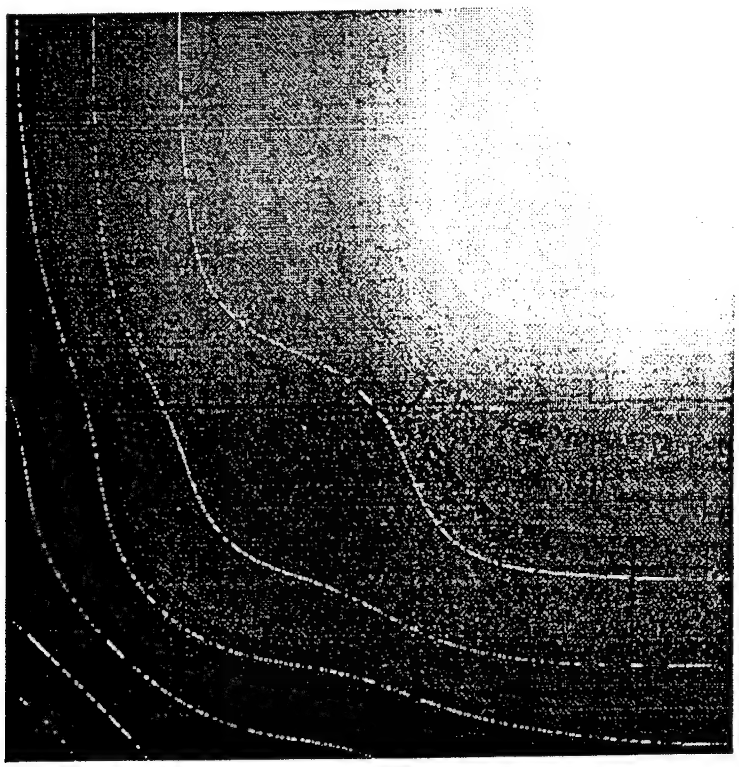

Fig 3 (b)   t=150

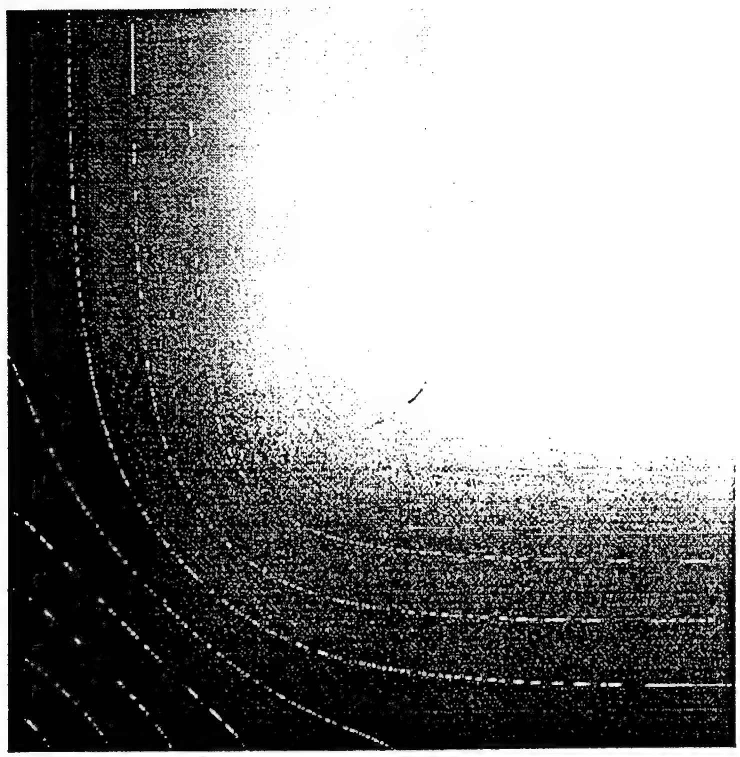

Fig 3(e) $t = 250$

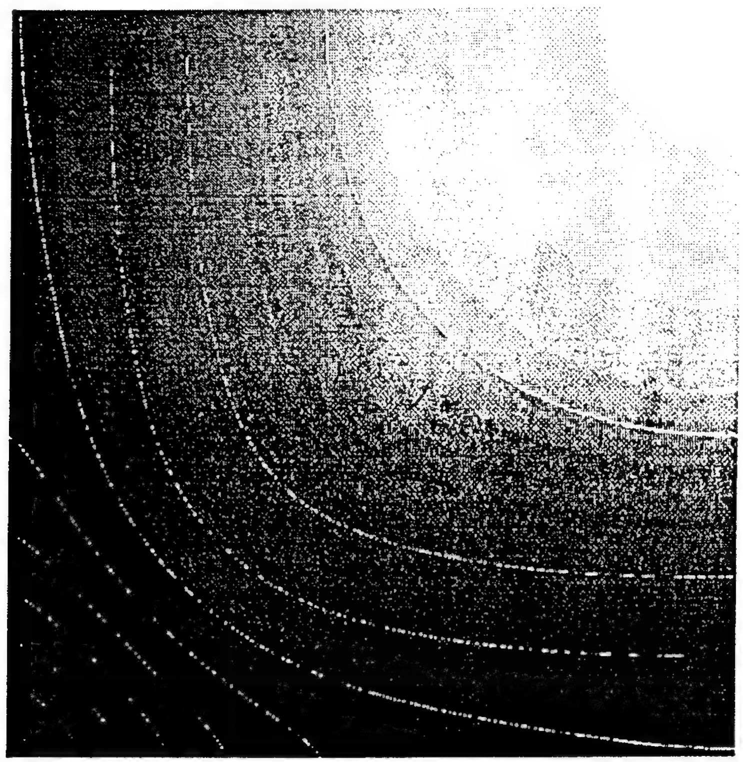

Fig 3(d) t=350

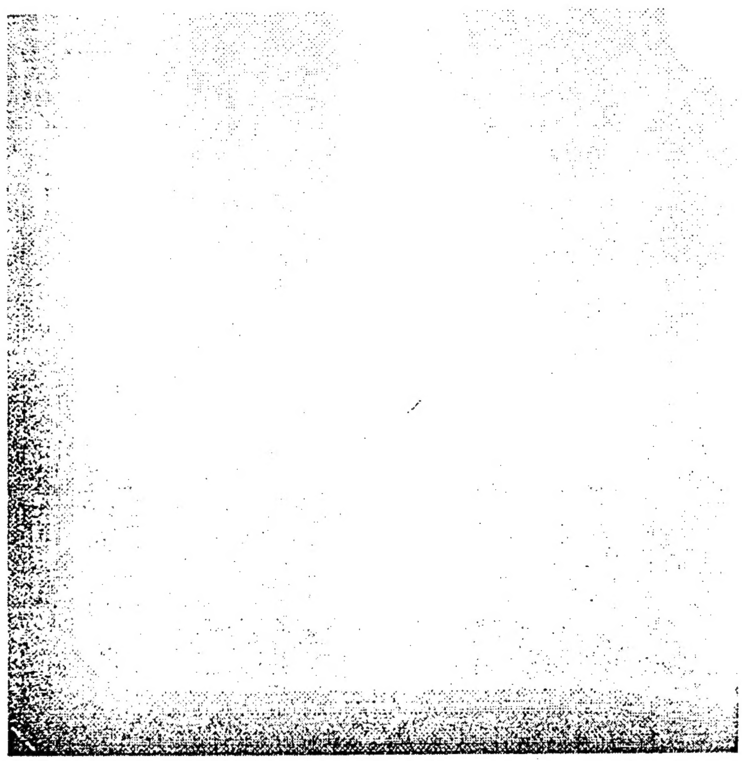

Fig 4(a) t = 50

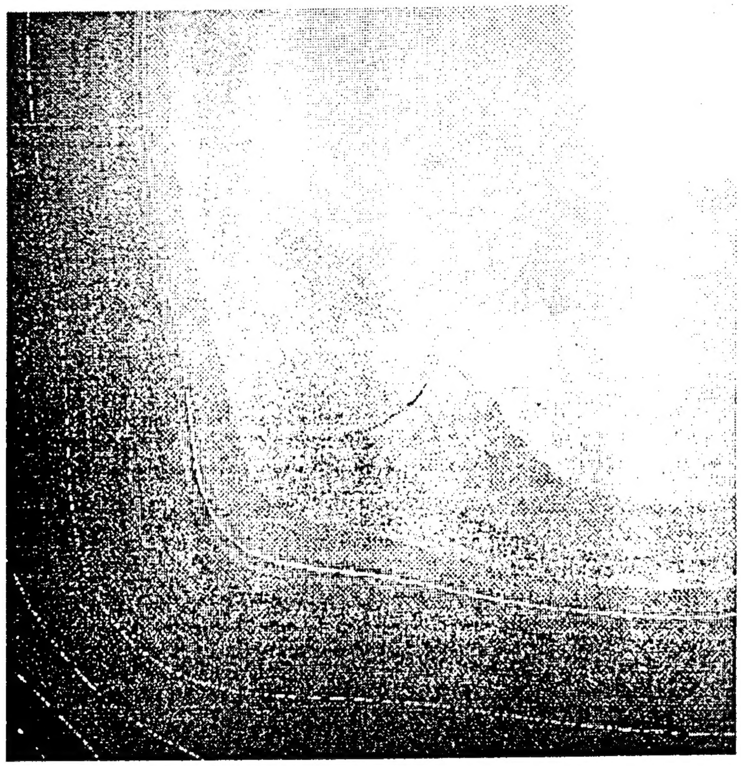

Fig 4 (b) t=150

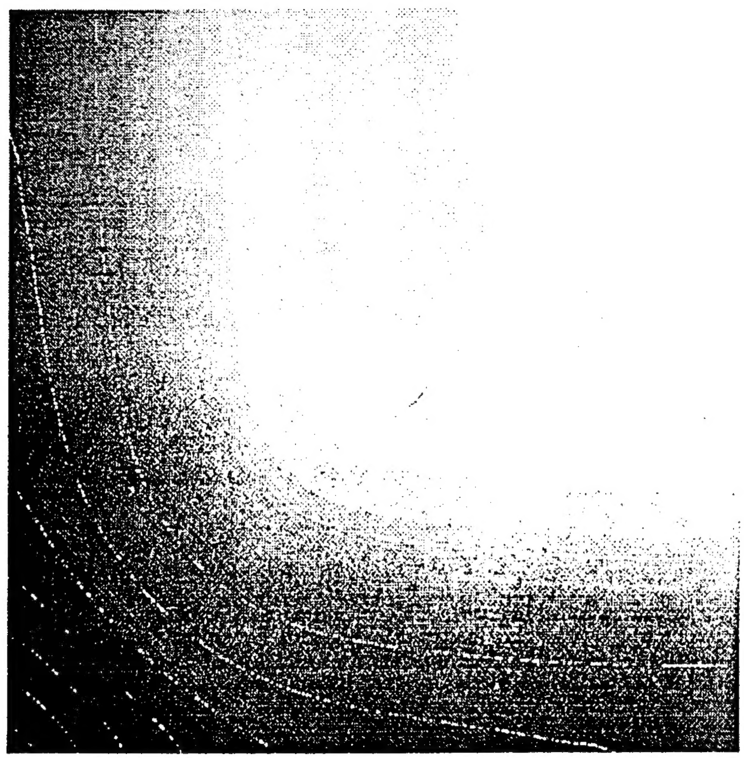

Fig 4 (c) $t = 250$

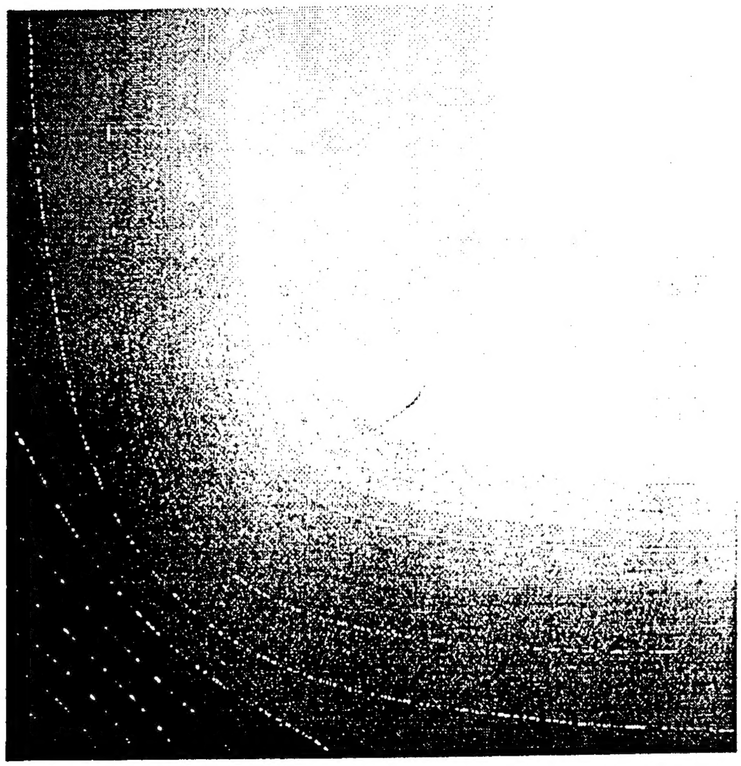

Fig 4(d) $t = 350$